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Multiscale Modeling of MEMS Dynamics and Failure

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This work studies multiscale phenomena in silicon micro-resonators which comprise the mechanical components of next-generation Micro-Electro-Mechanical Systems (MEMS). Unlike their larger relatives, the behavior of these sub-micron MEMS is not described well by conventional continuum models and finite elements, but it is determined appreciably by the interplay between physics at the Angstrom, nanometer and micron scales. As device sizes are reduced below the micron scale, atomistic processes cause systematic deviations from the behavior predicted by conventional continuum elastic theory. [1] These processes cause anomalous surface effects in the resonator frequency and quality factor–even for single crystal devices with clean surfaces due to thermal fluctuations.

The simulation of these atomistic effects is a challenging problem due to the large number of atoms involved and due to the fact that they are finite temperature phenomena. Our simulations include up to two million atoms in the device itself, and hundreds of millions more are in the proximal regions of the substrate. A direct, atomistic simulation of the motion of this many atoms is prohibitive, and it would be inefficient. The micron-scale processes in the substrate are well-described by finite elements, and an atomistic simulation is not required. On the other hand, atomistic processes in the device are inherently coupled to the micron-scale strain fields which extend out into the substrate. In order to capture physical effects at both length scales simultaneously, we have developed a multiple-scale simulation methodology. [2,3,4]

The computational technique applied here represents a significant departure from the usual finite element approach to MEMS modeling based on continuum elastic theory. When ordinary finite elements are refined to the atomic scale, the forces acting at the nodes do not resemble the true forces between atoms. Finite element models assume that the potential and kinetic energies are spread smoothly throughout each element. In reality, the potential energy is localized in covalent bonds and the kinetic energy is localized at the nuclei. Our multiscale approach uses finite elements in the peripheral regions where continuum elastic theory is valid, but it replaces finite elements with an atomistic model in regions of significantly anharmonic forces and large surface-area-to-volume ratios and where internal friction due to defects is anticipated. The different regions are joined seamlessly and run concurrently within a single simulation.

In this talk we present simulations of the vibrational behavior of micron-scale oscillators. We find anomalous surface effects that are due to atomistic processes, both in terms of temperature-dependent shifts of the resonant frequency and degradation of the quality factor (increased dissipation). Systematic experimental studies have seen anomalous dissipation at a somewhat larger scale where it has been attributed to surface degradation. [5,6,7] We also study the failure mechanisms in micro-resonators, which differ from those at large scale due to the instability of dislocations. These results are compared with the structural transitions seen in nanowire experiments. [8]

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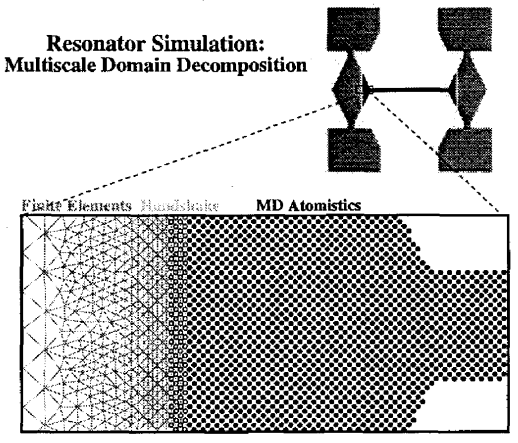
Topic: **Atomistics and Molecular Simulation**

Figure 1: Schematic illustration of Coupling of Length Scales for a long, thin micro-resonator. An atomistic simulation (MD) is used in the regions of the device undergoing significant oscillations, while finite elements (FE) is used in the peripheral regions where the strain fields extend out to the substrate. The two are joined through a consistent boundary condition in the handshaking region, and both are run concurrently in lock-step.



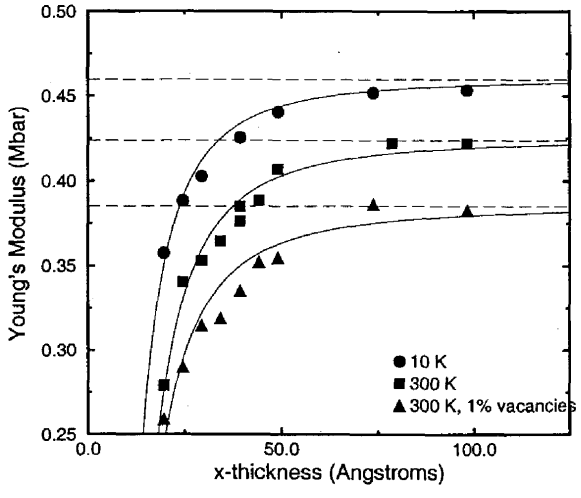


Figure 2: A plot of the Young's modulus as a function of the device size for a perfect crystal at two temperatures, T=10K and T=300K, and a crystal with 1% vacancies at T=300K. The dashed lines are the bulk value, and the solid curved line is a best fit to a modified constitutive equation including a term for atomistic surface effects.

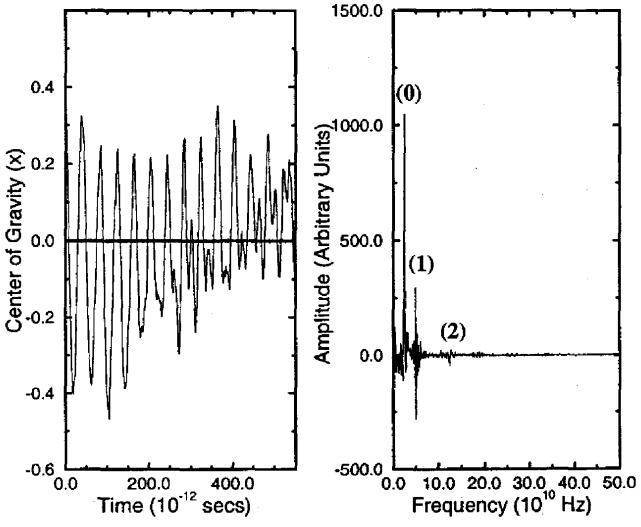


Figure 3: A plot of the oscillations and the corresponding frequency spectrum for a small (0.02 micron) resonator at room temperature. The device is initially excited in the fundamental mode (0). Appreciable components of the first (1) and second(2) harmonics have resulted from mode mixing due to anharmonic lattice effects.

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